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Simulation of surface topography with the method of movable cellular automata

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Abstract

Development of surface topography of two solids in a frictional contact is studied with the method of movable cellular automata. After the running-in process, the bodies are separated and the surface power spectra of both bodies are determined. The power spectra show a dependence on the wave vector, which is typical for fractal surfaces. It is shown, that roughness parameters of friction surface depend on relative velocity of sliding and external pressure.

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1. Introduction

The microscopic processes at the interface between two solids in friction involve very different processes both in the surface layers of solids (plastic deformation, storage of damages, detaching of wear particles and their repeated welding into the surfaces) and in the intermediate medium (lubrication fluids, wear particles, products of chemical reactions of the bulk material with atmosphere and lubricants). The intermediate medium has neither the properties of solids nor of the fluid and is usually referred to as a 'third body' [\[1,2\].](#page--1-0) The third body develops often in such a way that the minimum energy dissipation in friction is provided [\[3,4\].](#page--1-0)

In the present paper, we numerically investigate the formation of an intermediate layer between two solids in friction due to processes of plastic deformation, fracture and micro welding. For this purpose we use the method of Movable Cellular Automata—MCA. The MCA method allows to simulate such processes as plastic deformation, storage of micro damages and fracture, friction and wear, diffusion, adhesion, phase transformations and chemical reactions [\[5–8\]](#page--1-0).

The modeled system is represented in the MCA method as an assembly of discrete elements—'movable cellular automata'. The interactions of elements are defined in such a way that the isotropy of elastic properties is provided. Automata are characterized by the tensor of plastic deformation and the coupling state with their immediate neighbors. The parameter of the system are density, elastic constants, yield stress, fracture stress, fracture strain and viscosity.

The spatial evolution of movable automata is governed by the Newton–Euler equations of motion. This system contains both equations for translations and rotations:

$$
\begin{cases}\n m^i \frac{\mathrm{d}^2 \vec{R}^i}{\mathrm{d}t^2} = \sum_j (\vec{F}_n^{ij} + \vec{F}_\tau^{ij}) \\
\hat{J}^i \frac{\mathrm{d}^2 \vec{\theta}^i}{\mathrm{d}t^2} = \sum_j \vec{K}_r^{ij}\n\end{cases}
$$
\n(1)

 \vec{R}^i is radius vector; $\vec{\theta}^i$, rotation angle; m^i , mass and \hat{J}^i , moment of inertia of an automaton *i*. $\vec{F}^{\vec{y}}_n$ and $\vec{F}^{\vec{y}}_7$, normal and tangential force correspondingly. $\vec{K}^{\vec{y}}_7$, m force.

Each movable automaton is further characterized by a set of mechanical parameters corresponding to mechanical properties of the simulated material. The formalism of the movable cellular automata method is detailed described in

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Fig. 1. Simulated setup and external loading conditions: (a) structure and parameters of the setup, loading scheme; (b) loading velocity profile; (c) loading pressure profile.

the papers [\[9–12\].](#page--1-0) Due to mobility of automata and the possibility of switching the connection state of the neighbors, it is possible to simulate also destruction of old and formation of new surfaces profiles.

2. Numerical model

The simulated setup is shown in Fig. 1a. The diameter of automata was equal to 2.5 nm. The top block of the setup imitates the moving body, whereas the bottom block the body in rest. The coordinates of automata of the bottom layer of the bottom block have been fixed. The elements of the top layer of the top block were forced to move along the x-axis with velocity V_x (the time dependence of V_x is depicted in Fig. 1b). In a normal direction (along the y-axis), the upper layer of automata was subjected to force F_v , with time dependence as shown in Fig. 1c. In order to prevent the appearance of 'impact' effects connected with sharp changing of values of velocity or pressure, procedure of linear increasing of loading up to the certain value was used. For modeling an extended sample the periodic boundary conditions along the y-axis have been used.

Modeling of sliding friction in of contact area has been executed at various values of relative velocity of sliding and normal pressure ($v=2, 3, 4, 5$ m/s, $P=125, 255$ and 383 MPa which corresponds to $1/4$, $1/2 \pi$ 3/4 of yield stress).

3. Sample parameters

The material parameters used in the simulations correspond to the rail steel [\[13\]](#page--1-0). Stress–strain diagram of such material is presented on the Fig. 2. The automata parameters corresponding to the properties of the simulated material are presented in [Table 1.](#page--1-0) For transition of pair of interacting automata from a 'linked' state into a 'unlinked' state the criterion on the basis of calculation of stress intensity in the considered pair was used. This parameter was compared with the value of material strength; the criterion of transition can be written as:

$$
\sigma_{\text{int}}^{i(j)} \ge K^{ij} \sigma_s^i,\tag{2}
$$

or

$$
\sigma_{\text{int}}^{(i)} \ge K^{ij} \sigma_s^j. \tag{2a}
$$

Definition of characteristic material parameters

Fig. 2. Stress–strain diagram for rail steel.

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